A short note on the presence of spurious states in finite basis approximations

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Abstract

The genesis of spurious solutions in finite basis approximations to operators which possess a continuum and a point spectrum is discussed and a simple solution for identifying these solutions is suggested.

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Recently Ackad and Horbatsch[1] have presented a nice numerical method for the solution of the Dirac equation for the hydrogenic Coulomb problem using the Rayleigh-Ritz method[2]. Using a mapped Fourier grid method, a matrix representation of the Dirac Hamiltonian is constructed in a Fourier sine basis, which upon diagonalization yields reasonably numerically accurate eigenvalues for a mesh size which is not exceptionally large. Relativistic sum rules[3] provide a simple means of checking whether or not the number of basis states is adequate. As with any attempt to construct a matrix representation of an operator which contains continuum states, spurious states can occur and must be eliminated. Ackad and Horbatsch[1] have pointed out that in certain cases they can be identified by looking at the numerical structure of the large and small components of the corresponding eigenvector. Similar phenomenon occur in the mapped Fourier grid representation of the non-relativistic Schrödinger problem[4] in which non-physical roots are observed at random locations. Again the potentials considered support both bound as well as continuum states. The wave functions of these spurious states are characterized by their unphysical oscillations and non-vanishing amplitude in the classically forbidden regions. The authors point out that they have found no satisfactory mathematical explanation for the occurrence of these spurious levels.

In this note we wish to point out that the genesis of these spurious states can easily be understood and that there is a simple way to identify them. Consider an operator, $\hat{H}$, which possesses a continuum (or continua) as well as a point spectrum. The subspace spanned by its bound state eigenfunctions, $\mathcal{H}_{\mathcal{B}}$, is by itself certainly not complete. As the composition of this space is generally not known beforehand, a set of basis states which is complete and spans a space, $\mathcal{F}$, is chosen to construct a matrix representation of the operator, $\hat{H}$, to be diagonalized. Mathematically this corresponds to projecting the operator $\hat{H}$ onto the space $\mathcal{F}$. Clearly the eigenpairs obtained from diagonalizing the projected operator, $\hat{H}_P$, need not all be the same as those of the operator $\hat{H}$. However, because the set of basis states is complete, any state contained in $\mathcal{H}_{\mathcal{B}}$ can be expanded in terms of this set of basis states. Hence $\mathcal{H}_{\mathcal{B}}$ may also be regarded as a subspace of $\mathcal{F}$ and the complete diagonalization of $\hat{H}_P$ will yield not only the exact eigenstates of $\hat{H}$ but additional spurious eigensolutions. Note these spurious eigenfunctions are eigenfunctions of $\hat{H}_P$ but not of $\hat{H}$. Furthermore in this case the Rayleigh-Ritz bounds discussed in the paper by Krauthauser and Hill[2] apply now to the eigenstates of $\hat{H}_P$.

It is interesting to note that the same problem occurs in the Lanczos algorithm[5] when it is applied to operators which possess a bound state spectrum as well as a continuum[6]. This is not surprising as the Lanczos algorithm can also be considered as an application of the Rayleigh-Ritz method[7]. In this case an orthonormalized set of Krylov basis vectors is used to construct iteratively a matrix represention of the operator which is then diagonalized. Again spurious states can occur for precisely the same reasons given above. In this case we have proposed identifying the exact bound states in the following manner[6]. After each iteration, for each of the converging eigenpairs $(e_{l\lambda},|e_{l\lambda}\rangle)$, $\Delta_{l\lambda} = |e^2_{l\lambda} - < e_{l\lambda}|\hat{H}^2|e_{l\lambda} > |$ (where l is the iteration number) is calculated and a determination is made as to whether Δ is converging toward zero or not. For the exact bound states of $\hat{H}$, Δ must be identically zero while the other eigenstates states of the projected operator should converge to some non-zero positive value. This method has been successfully implemented to identify spurious states in non-relativistic[6] as well as relativistic[8] eigenvalue problems. A similar procedure can be implemented in any Rayleigh-Ritz application. One simply must check to see whether the eigensolutions from the diagonalization of $\hat{H}_P$ are also eigensolutions of $\hat{H}^2$.

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